Laurent Emmanuel Dardenne

List of Publications by Year
in descending order

49 papers	1,620 citations	394421 19 h-index	377865 34 g-index
50 all docs	50 docs citations	50 times ranked	2173 citing authors

#	Article	IF	Citations
1	Receptorâ€“ligand molecular docking. Biophysical Reviews, 2014, 6, 75-87.	3.2	324
2	Empirical Scoring Functions for Structure-Based Virtual Screening: Applications, Critical Aspects, and Challenges. Frontiers in Pharmacology, 2018, 9, 1089.	3.5	185
3	Highly Flexible Ligand Docking: Benchmarking of the DockThor Program on the LEADS-PEP Proteinâ€“Peptide Data Set. Journal of Chemical Information and Modeling, 2020, 60, 667-683.	5.4	144
4	A dynamic niching genetic algorithm strategy for docking highly flexible ligands. Information Sciences, 2014, 289, 206-224.	6.9	116
5	New machine learning and physics-based scoring functions for drug discovery. Scientific Reports, 2021, 11, 3198.	3.3	91
6	Design, synthesis and evaluation of novel feruloyl-donepezil hybrids as potential multitarget drugs for the treatment of Alzheimer's disease. European Journal of Medicinal Chemistry, 2017, 130, 440-457.	5.5	67
7	Drug design and repurposing with DockThor-VS web server focusing on SARS-CoV-2 therapeutic targets and their non-synonym variants. Scientific Reports, 2021, 11, 5543.	3.3	63
8	A multiple minima genetic algorithm for protein structure prediction. Applied Soft Computing Journal, 2014, 15, 88-99.	7.2	59
9	Design, synthesis and pharmacological evaluation of N -benzyl-piperidinyl-aryl-acylhydrazone derivatives as donepezil hybrids: Discovery of novel multi-target anti-alzheimer prototype drug candidates. European Journal of Medicinal Chemistry, 2018, 147, 48-65.	5.5	52
10	Structural modelling and comparative analysis of homologous, analogous and specific proteins from Trypanosoma cruzi versus Homo sapiens: putative drug targets for chagas' disease treatment. BMC Genomics, 2010, 11, 610.	2.8	45
11	A genetic algorithm for the ligand-protein docking problem. Genetics and Molecular Biology, 2004, 27, 605-610.	1.3	40
12	Novel series of tacrine-tianeptine hybrids: Synthesis, cholinesterase inhibitory activity, S100B secretion and a molecular modeling approach. European Journal of Medicinal Chemistry, 2016, 121, 758-772.	5.5	39
13	Electrostatic properties in the catalytic site of papain: A possible regulatory mechanism for the reactivity of the ion pair. Proteins: Structure, Function and Bioinformatics, 2003, 52, 236-253.	2.6	33
14	Investigation of the three-dimensional lattice HP protein folding model using a genetic algorithm. Genetics and Molecular Biology, 2004, 27, 611-615.	1.3	33
15	A new approach for potential drug target discovery through in silico metabolic pathway analysis using Trypanosoma cruzi genome information. Memorias Do Instituto Oswaldo Cruz, 2009, 104, 1100-1110.	1.6	27
16	Understanding the HIV-1 protease nelfinavir resistance mutation D30N in subtypes B and C through molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2010, 29, 137-147.	2.4	24
17	Structural modeling and docking studies of ribose 5-phosphate isomerase from Leishmania major and Homo sapiens: A comparative analysis for Leishmaniasis treatment. Journal of Molecular Graphics and Modelling, 2015, 55, 134-147.	2.4	23
18	Discovery of naphthylâ€Nâ€acylhydrazone p38Î± MAPK inhibitors with in vivo antiâ€inflammatory and antiâ€TNFâ€Î± activity. Chemical Biology and Drug Design, 2018, 91, 391-397.	3.2	22

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19	Design, synthesis, cholinesterase inhibition and molecular modelling study of novel tacrine hybrids with carbohydrate derivatives. Bioorganic and Medicinal Chemistry, 2018, 26, 5566-5577.	3.0	21
20	Critical Features of Fragment Libraries for Protein Structure Prediction. PLoS ONE, 2017, 12, e0170131.	2.5	20
21	Selection-Insertion Schemes in Genetic Algorithms for the Flexible Ligand Docking Problem. Lecture Notes in Computer Science, 2004, , 368-379.	1.3	19
22	Performance and parameterization of the algorithm Simplified Generalized Simulated Annealing. Genetics and Molecular Biology, 2004, 27, 616-622.	1.3	17
23	In silico identification of inhibitors of ribose 5-phosphate isomerase from Trypanosoma cruzi using ligand and structure based approaches. Journal of Molecular Graphics and Modelling, 2017, 77, 168-180.	2.4	17
24	Molecular docking study and development of an empirical binding free energy model for phosphodiesterase 4 inhibitors. Bioorganic and Medicinal Chemistry, 2006, 14, 6001-6011.	3.0	15
25	Design, Synthesis and Biological Evaluation of Novel Triazole N-acylhydrazone Hybrids for Alzheimerâ€™s Disease. Molecules, 2020, 25, 3165.	3.8	14
26	Synthesis of new lophineâ€“carbohydrate hybrids as cholinesterase inhibitors: cytotoxicity evaluation and molecular modeling. MedChemComm, 2019, 10, 2089-2101.	3.4	13
27	General Methodology to Optimize Damping Functions to Account for Charge Penetration Effects in Electrostatic Calculations Using Multicentered Multipolar Expansions. Journal of Physical Chemistry A, 2008, 112, 268-280.	2.5	11
28	Full-atom ab initio protein structure prediction with a Genetic Algorithm using a similarity-based surrogate model. , 2010, , .		10
29	A unique SaeS allele overrides cell-density dependent expression of saeR and lukSF-PV in the ST30-SCCmecIV lineage of CA-MRSA. International Journal of Medical Microbiology, 2016, 306, 367-380.	3.6	10
30	Analysis of Î±4 Î²1integrin specific antagonists binding modes: structural insights by molecular docking, molecular dynamics and linear interaction energy method for free energy calculations. Journal of the Brazilian Chemical Society, 2010, 21, 546-555.	0.6	7
31	LASSBioâ€1829 Hydrochloride: Development of a New Orally Active Nâ€Acylhydrazone IKK2 Inhibitor with Antiâ€inflammatory Properties. ChemMedChem, 2016, 11, 234-244.	3.2	7
32	Cinnamoyl-N-Acylhydrazone-Donepezil Hybrids: Synthesis and Evaluation of Novel Multifunctional Ligands Against Neurodegenerative Diseases. Neurochemical Research, 2020, 45, 3003-3020.	3.3	7
33	A multiobjective approach for protein structure prediction using a steady-state genetic algorithm with phenotypic crowding. , 2015, , .		6
34	Isobenzofuran-1(3H)-ones as new tyrosinase inhibitors: Biological activity and interaction studies by molecular docking and NMR. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2021, 1869, 140580.	2.3	6
35	Chiral Bistacrine Analogues: Synthesis, Cholinesterase Inhibitory Activity and a Molecular Modeling Approach. Journal of the Brazilian Chemical Society, 0, , .	0.6	5
36	Using Crowding-Distance in a Multiobjective Genetic Algorithm for Protein Structure Prediction. , 2016, , .		4

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37	MHOLline 2.0: Workflow for automatic large-scale modeling and analysis of proteins. Revista Mundi Engenharia Tecnologia E GestÃ£o (ISSN 2525-4782), 2023, 5, .	0.0	4
38	Genetic operators based on backbone constraint angles for protein structure prediction. , 2015, , .		3
39	Inserting Co-Evolution Information from Contact Maps into a Multiobjective Genetic Algorithm for Protein Structure Prediction. , 2018, , .		3
40	Estimating Protein Structure Prediction Models Quality Using Convolutional Neural Networks. , 2018, , .		3
41	Comparison of differential evolution variants for the molecular ligand-receptor docking problem. , 2015, , .		2
42	Molecular Dynamics Simulations of Cruzipains 1 and 2 at Different Temperatures. , 2007, , 158-162.		1
43	Improving de novo protein structure prediction using contact maps information. , 2017, , .		1
44	Using an aggregation tree to arrange energy function terms for protein structure prediction. , 2017, , .		1
45	Computational evaluation of natural compounds as potential inhibitors of human PEPCK-M: an alternative for lung cancer therapy . Advances and Applications in Bioinformatics and Chemistry, 2019, Volume 12, 15-32.	2.6	1
46	Expedient Microwave-Assisted Synthesis of Bis(n)-lophine Analogues as Selective Butyrylcholinesterase Inhibitors: Cytotoxicity Evaluation and Molecular Modelling. Journal of the Brazilian Chemical Society, 0, , .	0.6	1
47	Genetic Algorithm for Finding Multiple Low Energy Conformations of Poly Alanine Sequences Under an Atomistic Protein Model. , 2007, , 163-166.		1
48	Design, synthesis, and biological evaluation of new thalidomideâ€“donepezil hybrids as neuroprotective agents targeting cholinesterases and neuroinflammation. RSC Medicinal Chemistry, 0, , .	3.9	1
49	An Expedient Synthesis of Tacrine-Squaric Hybrids as Potent, Selective and Dualâ€‘Binding Cholinesterase Inhibitors. Journal of the Brazilian Chemical Society, 0, , .	0.6	0